Application and system benchmarks

High-Performance Computing System Administration

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Introduction

What are Benchmarks(Computing)?

- applications designed to characterize the performance of a system
- results can be used to compare and rank different systems
- to identify problems and monitor the progress of fixing them
  - check if the performance requested by the customer is actually achieved
- usually cannot fully characterize all performance aspects of a system
  - measure one specific metric (floating point operations, execution time,I/O operations...)
- to cover multiple metrics we have benchmark-suites
- many types of benchmarks (Algorithmic benchmarks, Parallel benchmarks,...)

Introduction

Benchmark Key Properties

1. **Relevance:** should measure important features.
2. **Representativeness:** should be broadly accepted by industry and academia.
3. **Equity:** all systems should be fairly compared.
4. **Repeatability:** results should be verifiable.
5. **Cost-effectiveness:** tests should be economical.
6. **Scalability:** tests should measure from single server to multiple servers
7. **Transparency:** Benchmark metrics should be readily understandable.

UEABS-Unified European Applications Benchmark Suite

- a set of currently 13 application codes taken from the pre-existing
  - PRACE and DEISA application benchmark suites
  - extended with the PRACE Accelerator Benchmark Suite
- providing a single benchmark suite of
  - currently relevant and publicly available application codes and datasets
  - a size which can realistically be run on large systems
- each application code has either one, or two input datasets
  - Test Case A is designed to run on Tier-1 sized systems
  - Test Case B is designed to run on Tier-0 sized systems
- current release is Version 2.2 (December 20, 2022)
- https://repository.prace-ri.eu/git/UEABS/ueabs

Example Benchmark

GPAW Description

A Projected Augmented Wave code

- electronic structure calculations based on
  - the density functional theory (DFT)
  - the time-dependent density functional theory (TD-DFT)
- DTF allows studies of ground state properties such as energetics and equilibrium geometries
- TD-DFT can be used for calculating excited state properties such as optical spectra
- written in Python and C and parallelized with MPI
- There is also a CUDA-based implementation for GPU systems

Example Benchmark

GPAW Dependencies and Installation

- C compiler with MPI support
- BLAS, LAPACK, BLACS and ScaLAPACK
- for GPAW 20.10.0 Python 3.6-3.9
- NumPy >=1.9
- SciPy >=0.14
- FFTW (Fastest Fourier Transform in the West), Libxc
- ASE (Atomic Simulation Environment)
- Installation choices
  - spack (py-gpaw)
  - manual with autoconf, Libtool and make

Example Benchmark

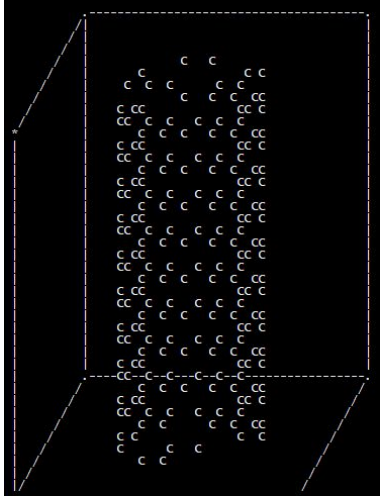
GPAW Datasets

1. Case A (small): Carbon nanotube
   a. ground state calculation for a carbon nanotube in vacuum
   b. scale up to 10 nodes and/or 100 MPI tasks
2. Case B (medium): Copper filament
   a. ground state calculation for a copper filament in vacuum
   b. scale up to 100 nodes and/or 1000 MPI tasks
3. Case C (large): Silicon cluster
   a. ground state calculation for a silicon cluster in vacuum
   b. scale up to 1000 nodes and/or 10000 MPI tasks

- result verification via 4 parameters including
  - expected number of Number of iterations
  - extrapolated energy

```
  ___ ___ ___ _ _ _
 |   |   |_  | | | |
 | | | | | . | | | |
 |__ |  _|___|_____|  21.1.0
 |___|_|

User:   hpctraining13@amp050
Date:   Thu Feb 16 16:27:23 2023
Arch:   x86_64
Pid:    402865
Python: 3.9.0
gpaw:   /usr/users/hpctraining13/.spack/0.17.1/install/haswell/gcc-9.3.0/py-gpaw-21.1.0-div4ac/lib/python3.9/site-packages/gpaw
_gpaw:  /usr/users/hpctraining13/.spack/0.17.1/install/haswell/gcc-9.3.0/py-gpaw-21.1.0-div4ac/lib/python3.9/site-packages/
        _gpaw.cpython-39-x86_64-linux-gnu.so
ase:    /usr/users/hpctraining13/.spack/0.17.1/install/haswell/gcc-9.3.0/py-ase-3.21.1-mqgcim/lib/python3.9/site-packages/ase (version 3.21.1)
numpy:  /usr/users/hpctraining13/.spack/0.17.1/install/haswell/gcc-9.3.0/py-numpy-1.21.3-amwali/lib/python3.9/site-packages/numpy (version 1.21.3)
scipy:  /usr/users/hpctraining13/.spack/0.17.1/install/haswell/gcc-9.3.0/py-scipy-1.7.1-vbxs7k/lib/python3.9/site-packages/scipy (version 1.7.1)
libxc:  4.3.4
units:  Angstrom and eV
cores: 100
OpenMP: False
OMP_NUM_THREADS: 1

Input parameters:
  convergence: {density: 0.01,
                eigenstates: 0.0001,
                energy: 0.001}
  eigensolver: rmm-diis
  h: 0.2
  maxiter: 16
  mixer: {backend: pulay,
          beta: 0.1,
          method: separate,
          nmaxold: 5,
          weight: 50}
  nbands: -60
  occupations: {fixmagmom: False,
                name: fermi-dirac,
                width: 0.1}
  poissonsolver: {eps: 1e-12,
                  name: fast,
                  nn: 3}

System changes: positions, numbers, cell, pbc, initial_charges, initial_magmoms

Initialize ...

C-setup:
  name: Carbon
  id: d60576a1f549371a163e72552ca58787
  Z: 6.0
  valence: 4
  core: 2
  charge: 0.0
  file: /home/uni08/hpctraining13/benchmark_project/ueabs/gpaw/gpaw_data/gpaw-setups-0.9.20000/C.LDA.gz
  compensation charges: gauss, rc=0.20, lmax=2
  cutoffs: 1.14(filt), 1.14(core),
  valence states:
                  energy  radius
    2s(2.00)   -13.639   0.635
    2p(2.00)    -5.414   0.635
    *s          13.573   0.635
    *p          21.797   0.635
    *d           0.000   0.635

  Using partial waves for C as LCAO basis

Reference energy: -244512.609073

Spin-paired calculation

Convergence criteria:
  Maximum total energy change: 0.001 eV / electron
  Maximum integral of absolute density change: 0.01 electrons
  Maximum integral of absolute eigenstate change: 0.0001 eV^2
  Maximum number of iterations: 16

Symmetries present (total): 4

  ( 1  0  0)  ( 1  0  0)  (-1  0  0)  (-1  0  0)
  ( 0  1  0)  ( 0  1  0)  ( 0 -1  0)  ( 0 -1  0)
  ( 0  0  1)  ( 0  0 -1)  ( 0  0  1)  ( 0  0 -1)
```

```
  Using the LDA Exchange-Correlation functional
  Interpolation: tri-quintic (5. degree polynomial)
  Poisson solver: FastPoissonSolver using
    6*3+1=19 point O(h^6) finite-difference Laplacian stencil;
    FFT axes: [2];
    FST axes: [0, 1].


Memory estimate:
  Process memory now: 94.34 MiB
  Calculator: 63.81 MiB
    Density: 3.43 MiB
      Arrays: 1.49 MiB
      Localized functions: 1.39 MiB
      Mixer: 0.54 MiB
    Hamiltonian: 1.09 MiB
      Arrays: 0.98 MiB
      XC: 0.00 MiB
      Poisson: 0.00 MiB
      vbar: 0.11 MiB
    Wavefunctions: 59.30 MiB
      Arrays psit_nG: 29.35 MiB
      Eigensolver: 29.63 MiB
      Projections: 0.13 MiB
      Projectors: 0.18 MiB

Total number of cores used: 100
Domain decomposition: 5 x 4 x 5

Number of atoms: 240
Number of atomic orbitals: 960
Number of bands in calculation: 540
Number of valence electrons: 960
Bands to converge: occupied

... initialized

Initializing position-dependent things.

Density initialized from atomic densities
Creating initial wave functions:
  540 bands from LCAO basis set
```



Example Benchmark

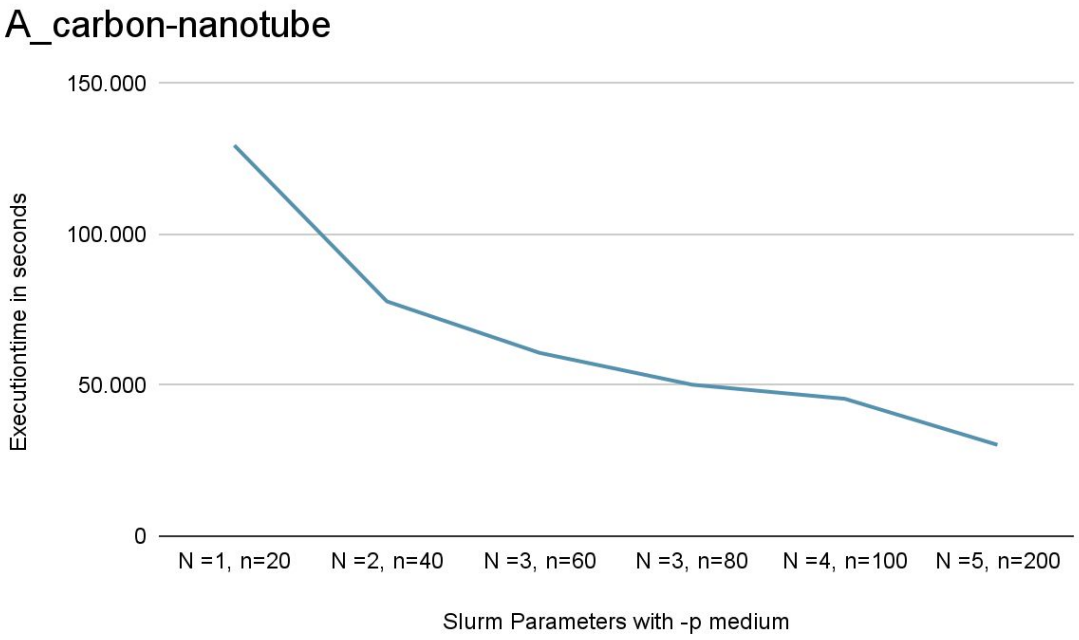
GPAW Example Output on dataset A_carbon-nanotube

```
#!/bin/bash
#SBATCH -p medium
#SBATCH -N 4
#SBATCH -n 100
#SBATCH -o job-%J.out

module purge
module load spack-user
source $SPACK_USER_ROOT/share/spack/setup-env.sh
spack load py-gpaw

srun gpaw python input.py
```

```
Result information:
  * Time:                    45.509 s
  * Number of iterations:    12
  * Dipole (3rd component): -115.165109
  * Fermi level:             -4.61200
  * Extrapolated energy:     -2397.625099
```

Example Benchmark

GPAW Example Output on dataset A_carbon-nanotube



References

- https://repository.prace-ri.eu/git/UEABS/ueabs
- https://hpc-wiki.info/hpc/Benchmarks
- https://en.wikipedia.org/wiki/Benchmark_(computing)#cite_note-5
- https://dberleant.github.io/papers/BenchmarkingContemporaryDeepLearningHardwareAndFrameworks.pdf